Computation of entropy increase for Lorentz gas and hard disks

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The H-theorem for dynamical systems:

Suppose that a transformation T on a phase space X has some invariant measure μ,

Suppose also that there is some mixing type mechanism of the approach to equilibrium for T, i.e. there is a sufficiently large family of non-equilibrium measures ν such that for all E,

$$\nu_t(E) =: \nu(T^{-t}E) \rightarrow_{t\rightarrow\infty} \mu(E)$$

The H-theorem means the existence of a <u>negative</u> entropy functional $S(\nu_t)$ which <u>increases monotonically</u> with t to zero, attained only for $\nu = \mu$.

Starting with the non-equilibrium initial measure ν, and partition formed with finite number of cells $\mathcal{P} = (\mathcal{P}_1, \mathcal{P}_2, \ldots, \mathcal{P}_n)$, then,

$$\nu_t(\mathcal{P}_i) = \nu \circ T^{-t}(\mathcal{P}_i)$$

is the probability at time t for the system to be in the cell $\mathcal{P}_i$.

The approach to equilibrium implies that

$$\nu_t(\mathcal{P}_i) \to \mu(\mathcal{P}_i)$$

as $t \to \infty$ for any i.

An entropy functional is defined as the relative entropy of the non-equilibrium measure ν_t with respect to μ for the observation $\mathcal{P}$

$$\mathcal{S}(t,\nu,\mathcal{P}) = -\sum_{i=1}^{n} \nu_t(\mathcal{P}_i) \ln(\frac{\nu_t(\mathcal{P}_i)}{\mu(\mathcal{P}_i)}) := -\mathcal{H}(t,\nu,\mathcal{P}) \tag{1}$$

The H-functional (1) is maximal when the initial distribution is concentrated on only one cell and minimal if and only if $\nu_t(\mathcal{P}_i) = \mu(\mathcal{P}_i), \forall i$.

A condition under which formula (1) shows a monotonic increase with respect to t is that the process $\nu_t(\mathcal{P}_i) = \nu \circ T^{-t}(\mathcal{P}_i)$ verifies the **Chapman-Kolmogorov** equation valid for Markov chains and also for other long memory chains.

For a dynamical system, this condition is hardly verified for given partition $\mathcal{P}$.

However, a very rapid mixing leads to the increase of the above entropy, at least during some initial stage, comparable with the relaxation stage in gas theory.

We compute the increase of such entropy functionals for some remarkable non-equilibrium distributions over the phase space of the Sinaï billiard.

The billiard is a hyperbolic system (with many singularity lines) and, in order to have a rapid mixing, we will consider initial distributions supported by the expanding fibers.

In billiard, the expanding fibers are approximated by colliding particles with parallel velocities. We call this class of initial ensembles **beams of particles**.

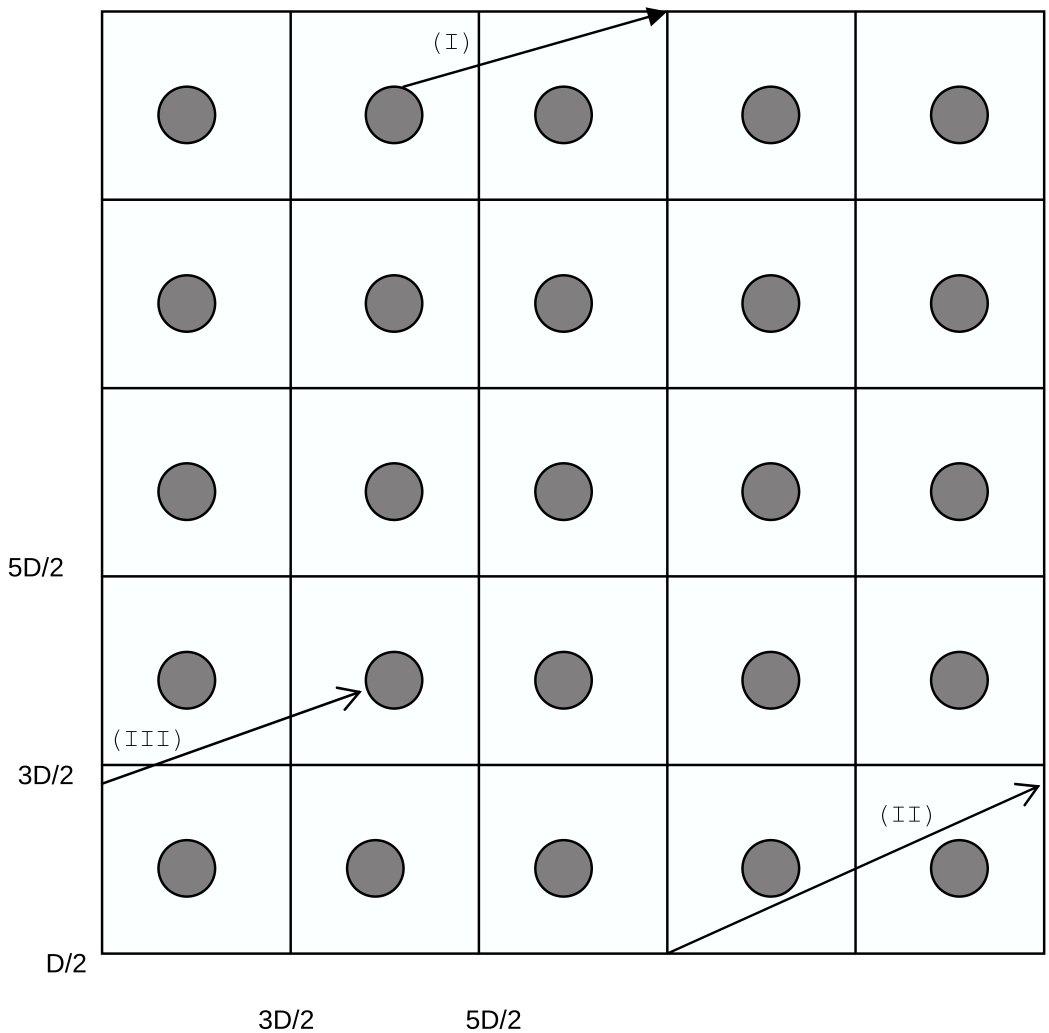


Figure 1: The motion of the particle on a toric billiard.

The Lorentz collision map

Discrete time dynamics on the set of all ingoing unitary velocity arrows $\mathbf{V}(P)$ at some point of the boundary of the disk.

To a colliding arrow $\mathbf{V}_1(P_1)$ at point P_1 on the boundary of the disk the map associates the next colliding arrow $\mathbf{V}_2(P_2)$ according to elastic reflection law.

The collision map does not take into account the free evolution between successive collisions.

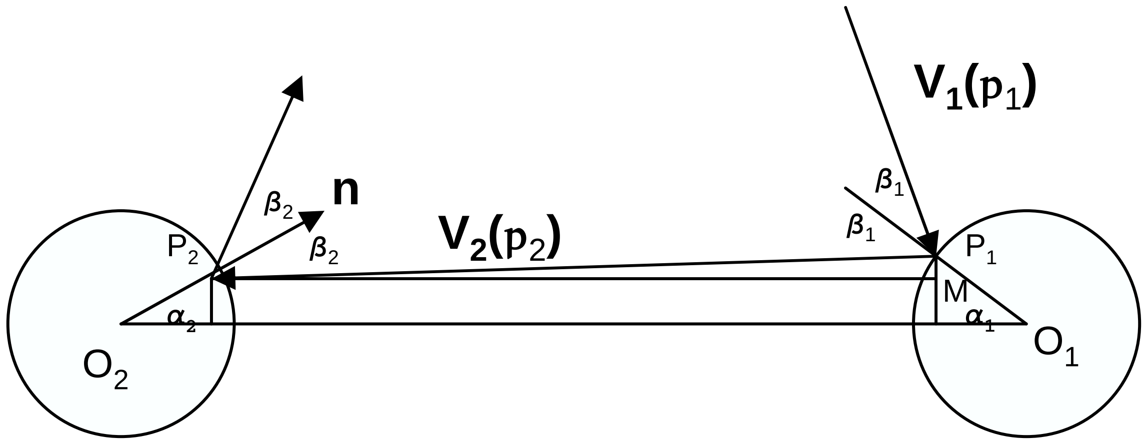


Figure 13: non-crossing Collision.

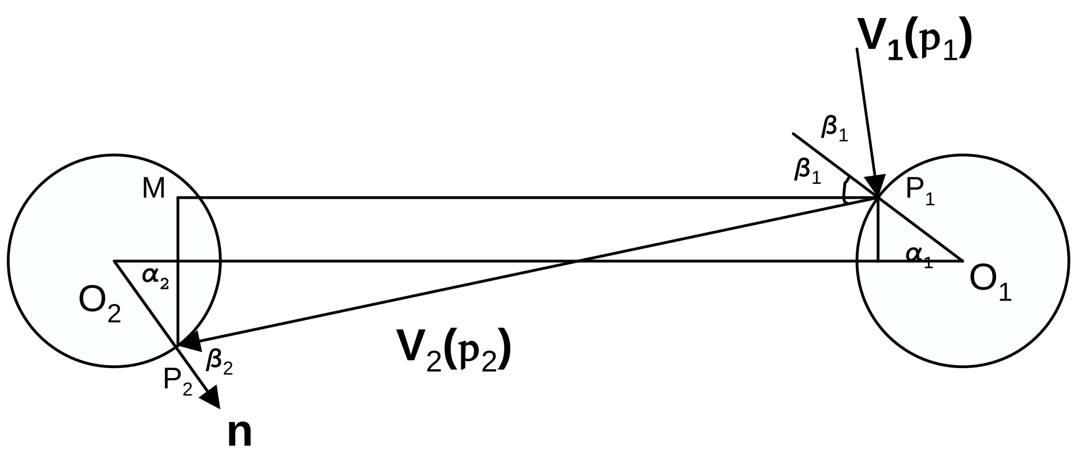


Figure 14: crossing Collision.

The phase space : two angles (β, ψ), where β is the angle between the outer normal at P and the incoming arrows $\mathbf{V}(P)$, $\beta \in [0, \frac{\pi}{2}[$, and $\psi \in [0, \pi]$ is the angle between x-axis and the outer normal at P. The collision map induces a map: $(\beta_1, \psi_1) \rightarrow (\beta_2, \psi_2)$

We used a uniform rectangular partition of the (β, ψ) space with the invariant measure:

$$\mu(\mathcal{P}_i) = \int_{\beta_i}^{\beta_{i+1}} \int_{\psi_i}^{\psi_{i+1}} \cos\beta d\beta d\psi \qquad (2)$$

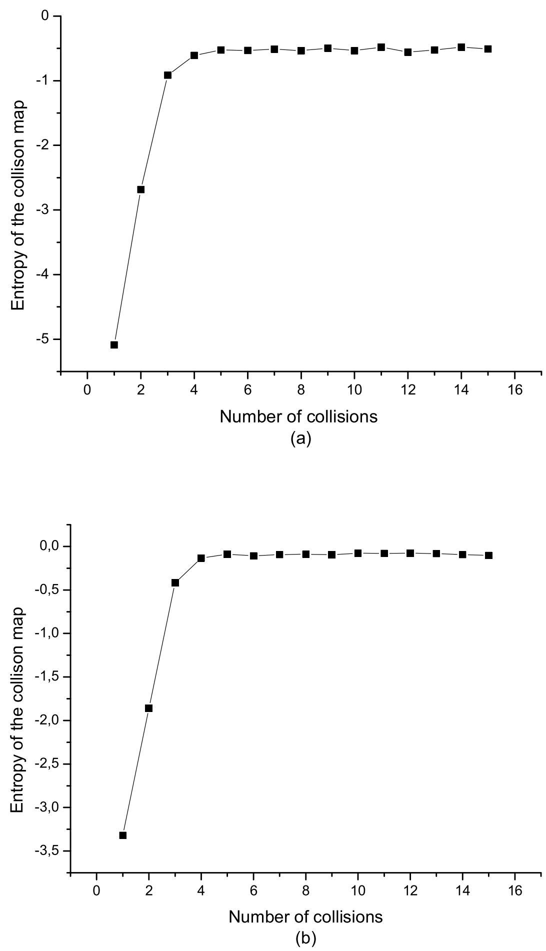


Figure 2: Entropy of the collision map versus number of collisions for (a) a beam of 640 particles for a radius a=0.2, neighboring disks centers distance 1 and a partition of (β, ψ) space into 25×25 cells, (b) a beam of 512 particles for the obstacles of radius 0.2, neighboring disks centers distance 1 and a partition of (β, ψ) space into 9×9 cells.

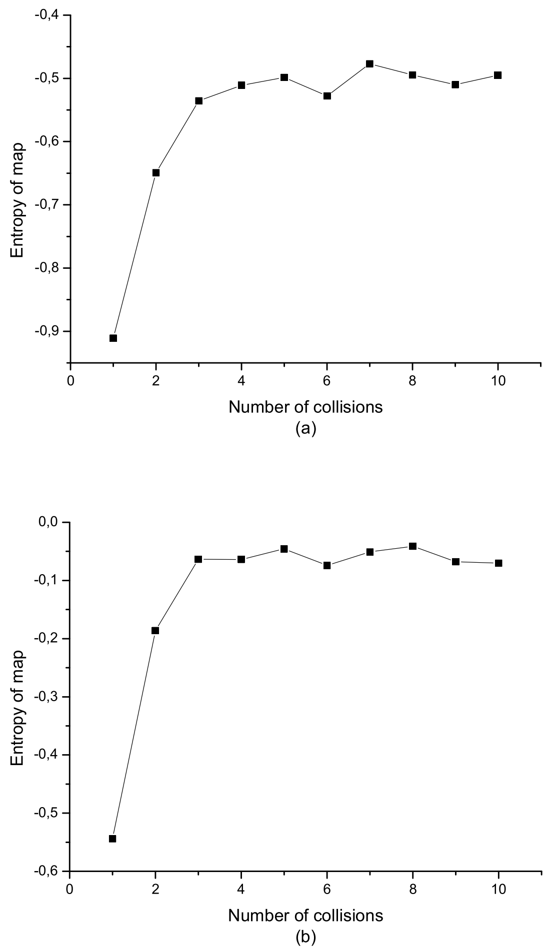


Figure 3: (a) and (b) are the entropy of the collision map with random initial conditions versus number of collisions for the system of particles of the Fig. 2, respectively.

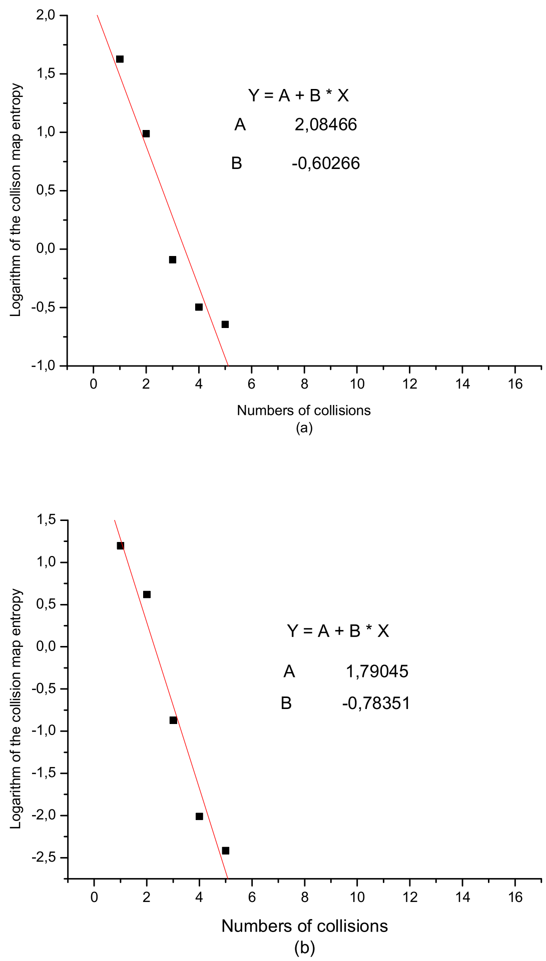


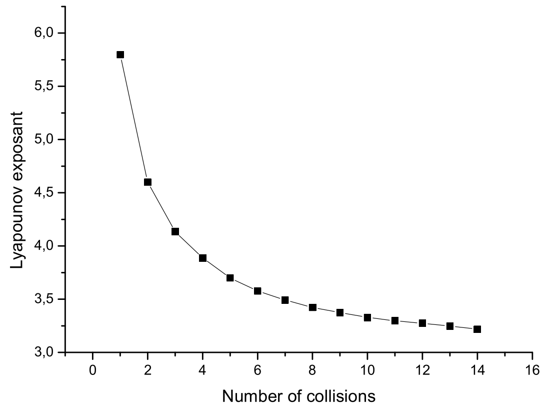
Figure 4: Logarithm of the collision map entropy versus number of collisions for the system of particles of the Fig. 2.

In order to compare the entropy increase as a function of the collision number with the entropy increase as a function of time, we compute the distribution of mean free time

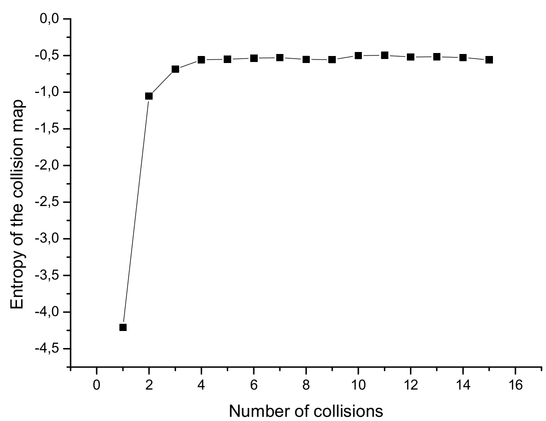
$\boxed{\text{Rate of increase and Lyapounov exponents}}$

$$\max(\mathcal{S}(k+1) - \mathcal{S}(k)) \equiv \triangle \mathcal{S} \leq \sum_{\lambda_i \geq 0} \lambda_i \qquad (3)$$

where the "max" is taken over k.



(a)



(b)

Figure 5: (a) Lyapounov exponent and (b) entropy of the collision map, versus of number of collisions for each particle. We see that the maximum of the entropy increase between two collisions is less than of the value of the Lyapounov exponent.

Spatially extended Lorentz gas entropy

N particles move in a large torus with n cells, in the center of each cell there is one disk. Initially the particles are distributed in only one cell followed until each executes t collisions with obstacles.

The probability that a particle is located in the ith cell is defined by:

$$\rho_i(t) = \frac{\text{Number of particles in cell } i \text{ having made } t \text{ collisions}}{N}$$

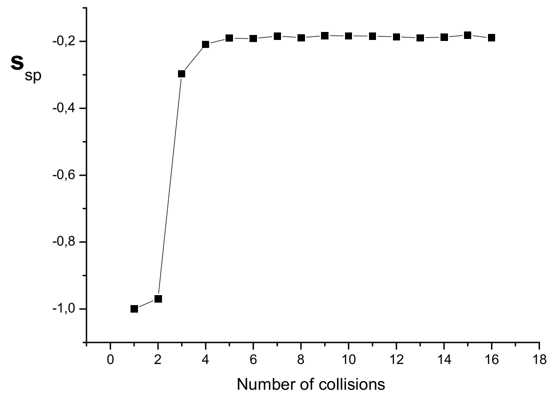
The equi-distribution is the equilibrium measure, $\mu_i = \frac{1}{n}$. The "space entropy" is defined by:

$$\mathcal{S}_{sp}(t) = -\sum_{i=1}^{n} \rho_i(t) \ln(\rho_i(t) n) \tag{4}$$

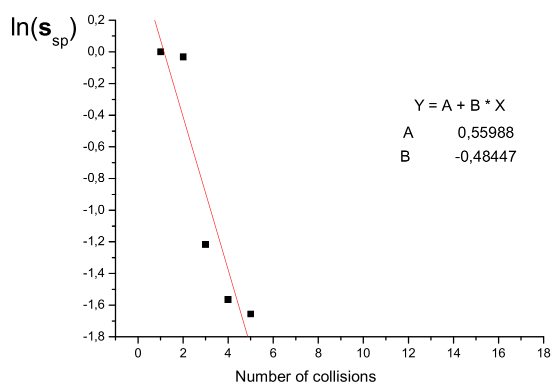
The maximum of absolute value of this entropy is equal to $-\ln n$.

The normalized space entropy is defined by:

$$\mathrm{s}_{sp}(t) = \frac{\mathcal{S}_{sp}(t)}{\ln n} \qquad (5)$$



(a)



(b)

Figure 8: (a) Normalized space entropy of the Lorentz gas versus number of collisions for a beam of 640 particles for obstacles of radius a=0.2, neighboring disks centers distance 1 and a partition of (x, y) space into 25×25 cells, (b) Logarithm of the space entropy versus number of collisions for this system.

Hard disks

N hard disks move in a large torus divided into n square cells. Initially the disks are distributed in only one cell, with random velocities.

Only binary collisions are considered.

The probability that a particle is located at time t in the ith cell is defined as above.

Define thenormalized sum of the positive Lyapounov exponents

$$\frac{1}{N}\sum_{\lambda_i>0}(\frac{\lambda_i}{\lambda_{max}})$$

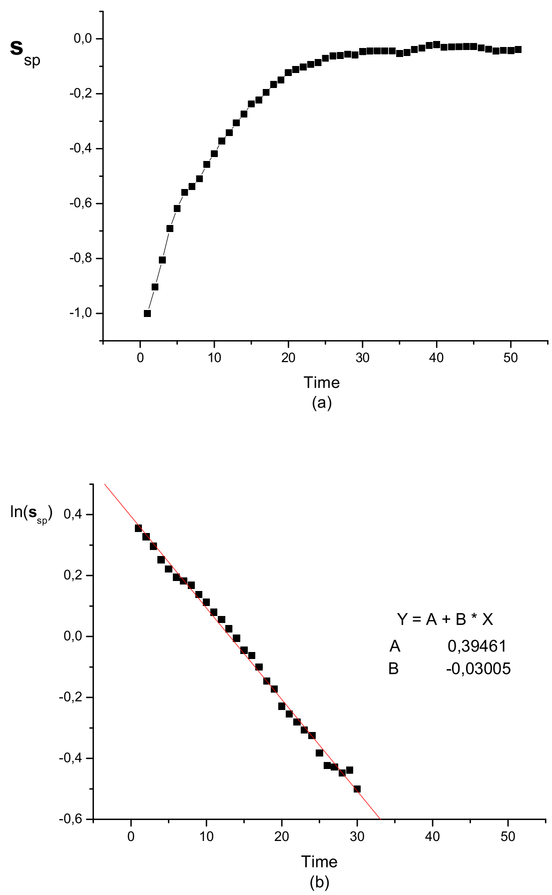


Figure 9: (a) Normalized space entropy and its monotonic part logarithm of the hard disks versus time for the 128 particles for the obstacles of radius a=0.05 which are initially localized in the first cell of (x, y) space with 6×6 cells and a density $\sigma_1 = 0.889$ disks per unit area.

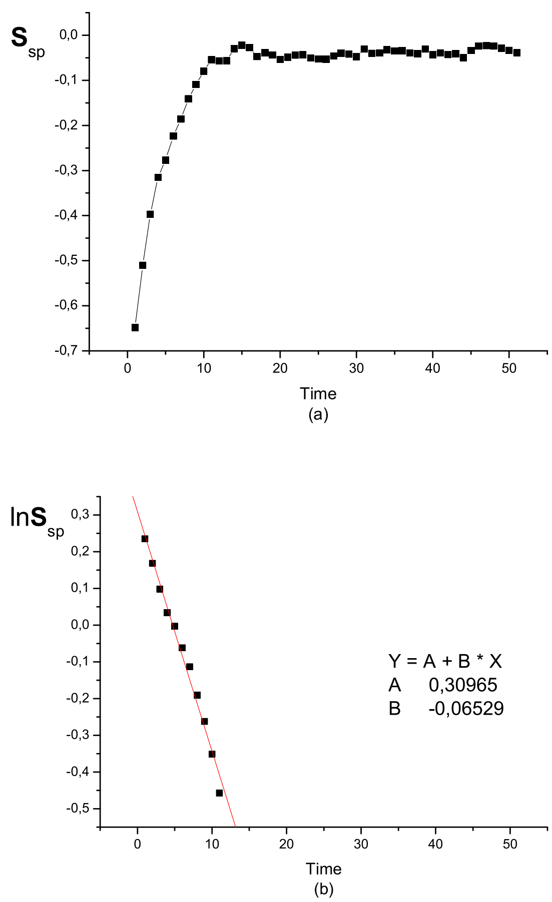


Figure 10: Normalized space entropy and its and its monotonic part logarithm for the same system as Fig. 9, with a density $\sigma_2 = 3.555$ disks per unit area.

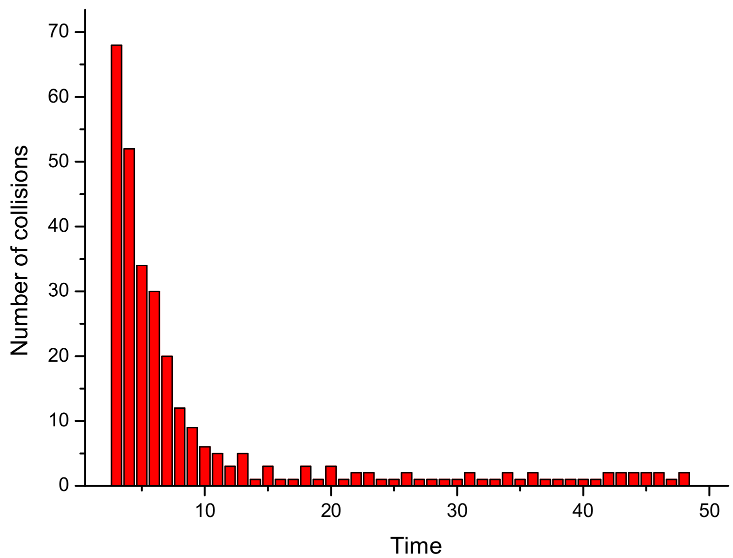


Figure 11: Number of collisions histogram system versus time in Fig. 9.

The computation shows that the inequality between the normalized entropy increase and the normalized sum of positive Lyapounov exponents is verified .

Density	$\frac{1}{N}\sum_{\lambda_i>0}(\frac{\lambda_i}{\lambda_{max}})$	$\triangle \mathbf{s}_{sp}$
3.555	0.367	0.139
0.889	0.294	0.115
0.222	0.239	0.144

Table 1: Hard disks systems of radius $a = 0.05$ with 6×6 cells, in terms of the density.